CONF-9008115--1

LA-UR--90-2268

DE90 015036

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AUG 0 6 1990

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TITLE **AN EVEN-PARITY/ODD-PARITY FORMULATION FOR DETERMINISTIC TRANSPORT CALCULATIONS ON MASSIVELY PARALLEL COMPUTERS (U)**

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AN EVEN-PARITY/ODD-PARITY FORMULATION FOR DETERMINISTIC TRANSPORT CALCULATIONS ON MASSIVELY PARALLEL COMPUTERS (U)

by

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Abstract: We have developed a highly parallel deterministic method for performing time-dependent particle (neutron, gamma-ray, or thermal radiation) transport calculations on arbitrarily connected 3-D tetrahedral meshes. The standard discrete-ordinates method, which is used to solve the first-order form of the transport equation, is extremely cumbersome to apply on such meshes and is based upon a mesh sweeping algorithm that is highly sequential in nature. A serial 1-D code for the CRAY-YMP and a parallel 1-D code for the CM-2 (Connection Machine) have been written to test our basic method. Comparisons between these two codes have shown that our new even/odd parity method is highly parallelizable.

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1. INTRODUCTION

Radiation transport plays a major role in many different technical areas including nuclear reactor design, controlled fusion research, atmospheric science, health and environmental safety analysis, and nuclear weapons design. The radiation transport equation can be expressed in the following form:[1]

$$\hat{\Omega} \cdot \nabla \psi + \sigma_t \psi = Q, \tag{1}$$

$$Q = \int\int \sigma_s (E' \to E, \hat{\Omega} \cdot \hat{\Omega}') \psi(\hat{\Omega}', E') d\hat{\Omega}' dE' + q, \tag{2}$$

where ψ denotes the angular flux, $\hat{\Omega}$ is a unit vector denoting the particle direction, E denotes the particle energy, σ_t denotes the total macroscopic interaction cross section, σ_s denotes the differential scattering cross section, and q denotes the inhomogeneous source function. The most common deterministic method for solving Eq. (1) is the

discrete–ordinates or S_n method.[1,2] This method is based upon the use of finite differences to approximate the spatial derivatives and quadrature methods to approximate the angular integrals appearing in this equation. The energy variable is discretized using the multigroup method, which can be thought of as a type of Galerkin method. The energy domain is partitioned into a set of intervals, and each interval corresponds to an energy group. The flux associated with an energy group is called the group flux and represents the total flux due to particles having energies within that group. When discretized, the left side of Eq. (1) takes the form of a lower triangular matrix, which allows ψ to be directly calculated given the source on the right side of Eq. (1). This gives rise to the standard iterative method for solving Eq. (1), which is called source iteration, and can be represented as follows:

$$\vec{\Omega} \cdot \vec{\nabla} \psi^{\ell+1} + \sigma_t \psi^{\ell+1} = Q^{\ell}, \tag{3}$$

where ℓ denotes the iteration index. Equation (3) represents the simplest form of source iteration, which corresponds to a Jacobi–type iteration. The most commonly used form of source iteration is related to a Gauss–Seidel method, and is composed of what is called inner iterations and outer iterations. It is not important to understand these iterations in detail. For our purposes it suffices to say that inner iterations involve only the source component resulting from transfers within a group, while outer iterations involve only the source component resulting from transfers between groups. The source iteration process is inherently sequential, and hence not suited to massively parallel computer architectures. Unfortunately, essentially all techniques developed to date for solving the transport equation require a source iteration at some point in the calculation. For instance the classic diffusion–synthetic scheme and recently developed multigrid schemes require a source iteration to attenuate high frequency error modes.[1,2,3]

1.1 DEVELOPMENT

As an alternative, we manipulate Eq. (1) into a form which is extremely amenable to parallel solution techniques. We begin by defining the even parity and odd parity fluxes, ψ^{+} and ψ^{-}, respectively,

$$\psi^{+}(\vec{\Omega}) \equiv \frac{\psi(\vec{\Omega}) + \psi(-\vec{\Omega})}{2}, \tag{4}$$

$$\psi^{-}(\vec{\Omega}) = \frac{\psi(\vec{\Omega})-\psi(-\vec{\Omega})}{2}, \tag{5}$$

It is not difficult to algebraically manipulate Eq. (1) into the following set of equations:

$$-\vec{\Omega}\cdot\vec{\nabla}\left(\frac{1}{\sigma_t}\vec{\Omega}\cdot\vec{\nabla}\psi^{+}\right)+\sigma_t\psi^{+}=Q^{+}-\vec{\Omega}\cdot\vec{\nabla}(Q^{-}/\sigma_t), \tag{6}$$

$$\psi^{-}=-\frac{1}{\sigma_t}\vec{\Omega}\cdot\vec{\nabla}\psi^{+}+\frac{1}{\sigma_t}Q^{-}. \tag{7}$$

$$-\vec{\Omega}\cdot\vec{\nabla}\left(\frac{1}{\sigma_t}\vec{\Omega}\cdot\vec{\nabla}\psi^{-}\right)+\sigma_t\psi^{-}=Q^{-}-\vec{\Omega}\cdot\vec{\nabla}(Q^{+}/\sigma_t), \tag{8}$$

$$\psi^{+}=-\frac{1}{\sigma_t}\vec{\Omega}\cdot\vec{\nabla}\psi^{-}+\frac{1}{\sigma_t}Q^{+}. \tag{9}$$

where the even–parity and odd–parity sources, Q^{+} and Q^{-} are defined in analogy with Eq. (4) and Eq. (5) respectively.

Equations (6) through (9) are redundant in that there are two equations each for ψ^{+} and ψ^{-}. However, they are not necessarily redundant when solved numerically. In particular, we have developed a finite–element formulation, based upon piecewise–linear and piecewise–constant trial spaces for 3–D tetrahedral meshes, such that Eqs. (6) and (7) are solved as a complete system to provide ψ^{+} at the tetrahedral nodes and ψ^{-} at the tetrahedral centers, while Eqs. (8) and (9) are solved as a complete system to provide ψ at the tetrahedral nodes and ψ^{+} at the tetrahedral centers. Interestingly, for almost all practical applications, one generally needs to know ψ^{-} only on the surface of the system because all quantities of physical interest in the interior of the system can be calculated from ψ^{+}. Furthermore, boundary conditions allow one to trivially calculate ψ^{-} from ψ^{+} at the outer boundary nodes. Thus, one need only solve Eqs. (6) and (7) to obtain all quantities of practical interest Consequently, we consider only this system of equations for the remainder of this discussion.

Solving Eqs. (6) and (7) using a standard source iteration scheme analogous to that used to solve Eq. (1), we obtain:

$$-\vec{\Omega}\cdot\vec{\nabla}\left(\frac{1}{\sigma_t}\vec{\Omega}\cdot\vec{\nabla}\psi^{+,\ell+1}\right)+\sigma_t\psi^{+,\ell+1}=Q^{+,\ell}-\vec{\Omega}\cdot\vec{\nabla}(Q^{-,\ell}/\sigma_t), \tag{10}$$

$$\psi^{-,\ell+1}=-\frac{1}{\sigma_t}\vec{\Omega}\cdot\vec{\nabla}\psi^{+,\ell+1}+\frac{1}{\sigma_t}Q^{-,\ell} \tag{11}$$

Note that the left side of Eq. (10) corresponds to a symmetric positive–definite, second–order operator that can be inverted using any technique developed for the standard diffusion operator (specifically, for our calculations, conjugate gradient with row and column scaling as a preconditioner).[4] Furthermore, once $\psi^{+,\ell+1}$ has been obtained from Eq. (10), $\psi^{-,\ell+1}$ can be explicitly obtained without a matrix inversion.

We have performed a fourier analysis which indicates that this form of source iteration has error attenuation properties very similar to those of the standard form, Eq. (3). However, unlike the standard form, this new form is extremely compatible with massively parallel computer architectures. Furthermore, it appears that highly efficient acceleration schemes such as the diffusion–synthetic scheme for inner iteration acceleration, and the linear–multifrequency–grey scheme[5] for outer iteration acceleration, can be easily applied to Eqs. (6) and (7) on complicated meshes, whereas great difficulties arise in applying such schemes to Eq. (1) on such meshes. One of the major deficiencies of modern numerical transport methods is a lack of effective acceleration schemes for these types of calculations. Thus, the approach that we have outlined has the potential for significantly advancing the state–of–the–art for transport calculations on complicated 3–D meshes through the exploitation of massively parallel computing techniques.

1.2 RESULTS

A 1–D one energy group time–dependent slab–geometry version of the new even–parity and odd–parity transport equations has been coded for both the CRAY–YMP and the CM–2 (Connection Machine).[6–9] Both versions use basic source iteration with two–moment diffusion–synthetic acceleration of the inner iterations along with standard S_n angular discretization and linear continuous finite element spatial discretization (with lumping of removal and source terms).

We present computational results for two problems. Each figure will be comparing execution times (as the number of mesh cells is varied) between the CRAY–YMP version and the parallel CM–2 version. The CM–2 or Connection Machine we use has 64K (or 65536) bit serial processors each with 32K bytes of memory, 64–bit floating–point Weitek chips, and 10 gigabytes disk storage.

The first problem is a S_{16}, steady–state calculation with constant width mesh cells, vacuum boundaries, and a flat source across the spatial domain. In both the CRAY–YMP version and the CM–2 version we set the number of source iterations, set the number of conjugate gradient iterations, and then varied the number of mesh cells while comparing execution times between the two versions. These results are shown in Fig. 1. For these results only 32K processors (or half the machine) were used on the CM–2, and one cpu on the CRAY–YMP. It may be seen that the parallelized CM–2 version performs better than the CRAY–YMP version for all number of mesh cells. Specifically, at 225,000 mesh cells the CM–2 version is approximately 2 times faster. Also, note that the CRAY–YMP curve is extrapolated after 111,000 mesh cells since the problem size exceeded the CRAY's available memory.

The second problem is a S_2, time–dependent calculation, with vacuum boundaries, and a flat unit source across the spatial domain. For this problem we set the width of the spatial domain to 50 mfp. The macroscopic scattering cross–sections zeroeth moment is set at 2, and the first moment at 1. The macroscopic absorption cross–section is equal to 1 and there is no fission. For the results shown in Fig. 2 at each number of mesh cells we performed a time–dependent calculation with the time step set at .005 sec and 10 steps. For each number of mesh cells we performed this time–dependent calculation and compared execution times between the CRAY–YMP and CM–2 versions. For these calculations we used all 64K processors on the CM–2, and 1 cpu on the CRAY–YMP. The parallelized CM–2 version performs better than the CRAY–YMP version for all number of mesh cells. Specifically, at 200,000 mesh cells the CM–2 version is approximately 4 times faster. Again, note that the CM–2 had no difficulty handling problem sizes larger than 250,000 mesh cells whereas the problem size got too large for the CRAY–YMP at approximately 200,000 mesh cells.

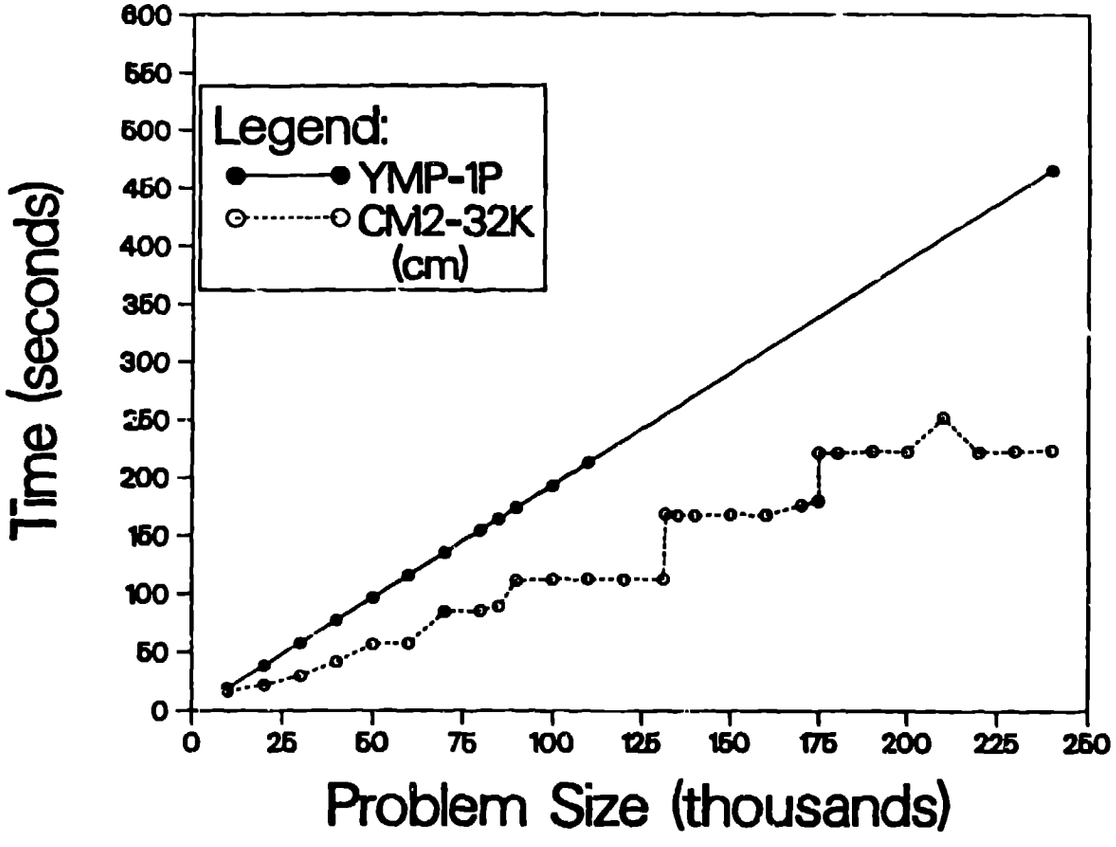
Time (seconds)
Problem Size (thousands)
Legend:
YMP-1P
CM2-32K
(cm)
0
50
100
150
200
250
300
350
400
450
500
550
600
0
25
50
75
100
125
150
175
200
225
250

FIG. 1.

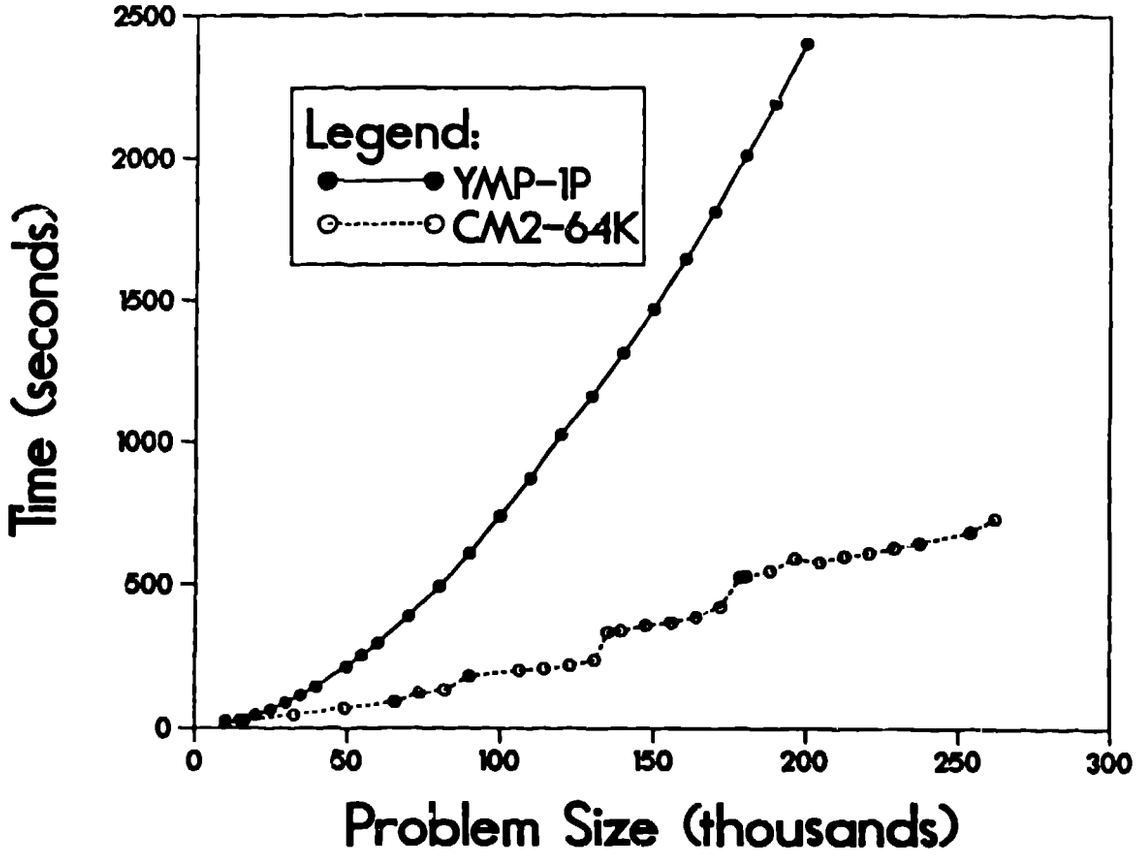
Legend:
YMP-1P
CM2-64K
Time (seconds)
Problem Size (thousands)
0
500
1000
1500
2000
2500
0
50
100
150
200
250
300

FIG. 2.

2. CONCLUSIONS

In conclusion, standard discrete–ordinates, or S_n, is based upon a mesh sweeping algorithm that is highly sequential in nature thus not suited to massively parallel computer architectures. Our new even–parity/odd–parity method is highly parallelizable as seen from the results presented.

The even–parity equation has been solved with isotropic scattering and S_n angular discretization.[10] However, with isotropic scattering the odd–parity doesn't appear in the even–parity equation. Thus, with isotropic scattering, one need not solve the odd–parity equation.

Our method is "new" in that we are simultaneously solving the discretized 2nd–order form of the even–parity transport equation and the discretized 1st–order form of the odd–parity transport equation assuming anisotropic scattering and using source iterations with two–moment diffusion synthetic acceleration. The basic discretized equations are obtained by employing an S_n–like discretization in direction together with a linear–continuous finite–element discretization (with lumping of the removal and source terms) in space.

The diffusion–like equation for the even–parity flux is a major advantage for our new method since much work has been done on parallel solution algorithms for the diffusion equation (specifically conjugate gradient with row and column scaling). Another major advantage is the direct solution of the odd–parity equation; two diffusion matrices do not have to be solved during each source iteration.

Many factors need to be investigated for 3–D multigroup calculations such as generalizing linear multifrequency–grey to treat neutronics calculations with fission and downscatter. Also, for 3–D parallel calculations on the CM–2, we need to develop optimal data storage and retrieval schemes, optimal iteration matrix and source vector generation schemes, and an optimal conjugate gradient solver. Ultimately, we will have a state–of–the–art multigroup, time–dependent parallel transport solver for neutron, gamma–ray, or thermal radiation calculations on complicated 3–D tetrahedral meshes.

3. REFERENCES

1. E. E. Lewis., W. F. Miller., JR., Computational Methods of Neutron Transport, John Wiley & Sons, Inc., New York, (1984).

2. J. E. Morel., "Synthetic Acceleration Method for Discrete Ordinate Calculations with Highly Anisotropic Scattering," Nuclear Science and Engineering, Vol. 82, p. 34, (1982).

3. A. Barnett, J. E. Morel, D. R. Harris, "A Multigrid Acceleration Method For The One–Dimensional S_n Equations with Anisotropic Scattering," Nuclear Science and Engineering, Vol. 102, p. 1, (1989).

4. H. C. Elman, "Iterative Methods for Large, Sparse, Nonsymmetric Systems of Linear Equations," University Microfilms International, Ann Arbor, MI., Yale University, (1982).

5. J. E. Morel., E. W. Larsen., M. K. Matzen., "A Synthetic Acceleration Scheme for Radiative Diffusion Calculations," Journal of Quantitative Spectroscopy and Radiative Transfer (JQSRT), Vol. 34, p. 243, (1985).

6. Connection Machine Model CM–2 Technical Summary, Version 5.1, Thinking Machines Corporation, Cambridge, Mass., (May 1989).

7. CM Fortran User's Guide, Version 5.2–0.6, Thinking Machines Corporation, Cambridge, Mass., (September 1989).

8. CM Fortran Reference Manual, Version 5.2–0.6, Thinking Machines Corporation, Cambridge, Mass., (September 1989).

9. Getting Started in CM Fortran, Version 5.2–0.6, Thinking Machines Corporation, Cambridge, Mass., (February 1990).

10. L. L. Briggs., W. F. Miller., JR., E. E. Lewis., "Ray–Effect Mitigation in Discrete Ordinate–Like Angular Finite Element Approximations in Neutron Transport," Nuclear Science and Engineering, Vol. 57, p. 205, (1975).